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INTRODUCTION TO THE THERMODYNAMICS OF SPIN CHAINS *

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ABSTRACT

We review how to obtain the thermodynamic Bethe Ansatz (TBA) equations for the antiferromagnetic Heisenberg ring in an external magnetic field. We review how to solve these equations for low temperature and small field, and calculate the specific heat and magnetic susceptibility.

1. Motivation

Quantum spin chains provide some of the simplest examples of physical systems with quantum-algebra[!!!!] symmetry. A well-known example is the open quantum spin chain consisting of N spins with the Hamiltonian

$$\mathcal{H} = \sum_{k=1}^{N-1} \left\{ \sigma_k^1 \sigma_{k+1}^1 + \sigma_k^2 \sigma_{k+1}^2 + \frac{1}{2}(q + q^{-1}) \sigma_k^3 \sigma_{k+1}^3 \right\} - \frac{1}{2}(q - q^{-1}) \left(\sigma_1^3 - \sigma_N^3 \right) , \tag{1.1}$$

where $\vec{\sigma}$ are the usual Pauli matrices, and q is an arbitrary complex parameter. This model is[!!!!,!!!!] integrable and the Hamiltonian commutes[!!!!,!!!!] with the generators of the quantum algebra $U_q[su(2)]$.

This model can be generalized in various directions. We have considered integrable open chains with quantum-algebra symmetry that have instead spins in

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higher-dimensional representations[!!!!], or spins in the fundamental representation of larger symmetry algebras[!!!!]. (See also Ref. !!!!.)

We would like to determine the physical properties (e.g., low-temperature magnetic susceptibility and specific heat) of such models for $|q| = 1$ in the thermodynamic ($N \to \infty$) limit. For the model (1.1), some steps in this direction have already been taken in Ref. !!!!. Because these models are integrable, the spectra of their Hamiltonians are known implicitly through the Bethe Ansatz (BA) equations. Unfortunately, this is still quite far from determining the models' physical properties.

We consider here instead, as a warm-up exercise, the analogous problem for the antiferromagnetic Heisenberg ring, with Hamiltonian

$$\mathcal{H} = \frac{1}{4} \sum_{k=1}^{N} (\vec{\sigma}_k \cdot \vec{\sigma}_{k+1} - 1) - \frac{H}{2} \sum_{k=1}^{N} \sigma_k^3 \,, \qquad \vec{\sigma}_{N+1} = \vec{\sigma}_1 \,, \tag{1.2}$$

where $H (\geq 0)$ is an external magnetic field. Although this model is comparatively simpler, the methods used to investigate it can presumably also be used to study integrable chains with quantum-algebra symmetry.

The low-temperature thermodynamics of this model was determined approximately twenty years ago as the result of the work of many people: Yang and Yang[!!!!], Takahashi[!!!!], Gaudin[!!!!], Johnson and McCoy[!!!!], *et al.* The fact that this work (certain details of which have never been published) is scattered among many papers contributed to the difficulty we experienced in learning about it.

We summarize this work here, in the hope of making it more accessible to others. Following Takahashi, we formulate in Section 2 the so-called thermodynamic Bethe Ansatz (TBA) equations for the antiferromagnetic Heisenberg ring. These are an infinite set of coupled nonlinear integral equations, which describe the equilibrium thermodynamics of the model at temperature T and in the field H. Following Johnson and McCoy, in Section 3 we solve the TBA equations in a systematic low-T and small-H perturbative expansion; and we calculate the free energy, specific heat, and magnetic susceptibility.

We warn the reader that we shall encounter along the way several arguments that are far from rigorous. Nevertheless, as far as we know, this is still the present state of the art.

While there are other ways[!!!!,!!!!] of calculating the low-temperature specific heat within the general TBA approach, the method pursued here has the merit of treating this calculation in the same manner as the one for the magnetic susceptibility.

Review articles on the thermodynamics of integrable models which we have found particularly useful are Refs. !!!! - !!!!.

2. TBA equations

The Hamiltonian for the antiferromagnetic Heisenberg ring in a magnetic field is given by Eq. (1.2). The corresponding energy eigenvalues, which can be determined by either the coordinate!!!!, algebraic!!!!, or analytic!!!! Bethe Ansatz, are given by

$$E = -\frac{1}{2}\sum_{\alpha=1}^{M} \frac{1}{\lambda_\alpha^2 + \frac{1}{4}} - H\left(\frac{N}{2} - M\right) , \tag{2.1}$$

where the variables $\{\lambda_\alpha\}$ satisfy the Bethe Ansatz (BA) equations

$$\left(\frac{\lambda_\alpha + \frac{i}{2}}{\lambda_\alpha - \frac{i}{2}}\right)^N = -\prod_{\beta=1}^{M} \frac{\lambda_\alpha - \lambda_\beta + i}{\lambda_\alpha - \lambda_\beta - i} , \qquad \alpha = 1, \cdots, M , \qquad M \le \frac{N}{2} . \tag{2.2}$$

These equations can be written more compactly as

$$\left[e_1(\lambda_\alpha)\right]^N = -\prod_{\beta=1}^{M} e_2(\lambda_\alpha - \lambda_\beta) , \tag{2.3}$$

where

$$e_n(\lambda) \equiv \frac{\lambda + \frac{in}{2}}{\lambda - \frac{in}{2}} . \tag{2.4}$$

These equations are difficult to solve for finite N. Fortunately, in the physically-interesting thermodynamic ($N \rightarrow \infty$) limit, these equations become easier to solve. Indeed, one then finds (see, e.g., Ref. !!!!) that the BA equations have "string" solutions. For instance, a string of length 1 is

$$\lambda^{(1)} = x ,$$

where x is an arbitrary real number, which is called the "center" of the string. Moreover, a string of length 2 is

$$\left\{ \begin{array}{l} \lambda^{(1)} = x + \frac{i}{2} \\ \lambda^{(2)} = x - \frac{i}{2} \end{array} \right. ,$$

a string of length 3 is

$$\begin{cases} \lambda^{(1)} = x + i \\ \lambda^{(2)} = x \\ \lambda^{(3)} = x - i \end{cases},$$

and so on. We adopt the "string hypothesis" which states that *all* the solutions $\{\lambda_\alpha\,, \alpha = 1, \cdots, M\}$ organize themselves into such strings. That is, the solutions are collections of M_n strings of length n of the form

$$\lambda_\alpha^{(n,j)} = \lambda_\alpha^n + i\left(\frac{n+1}{2} - j\right), \tag{2.5}$$

where $j = 1, \cdots, n$; $\alpha = 0, 1, \cdots, M_n$; $n = 1, \cdots, \infty$; and the centers λ_α^n are real. A particular solution of the BA equations corresponds to a set of non-negative integers $\{M_n\}$ and the M_n real numbers λ_α^n for each n. Observe that the total number of λ variables, and BA equations, is $M = \sum_{n=1}^\infty nM_n$.

Under this hypothesis, the BA equations (2.3) become

$$\left[e_1(\lambda_\alpha^{(n,j)})\right]^N = -\prod_{m=1}^\infty \prod_{\beta=0}^{M_m} \prod_{k=1}^m e_2(\lambda_\alpha^{(n,j)} - \lambda_\beta^{(m,k)})\,. \tag{2.6}$$

Following Takahashi!!!! and Gaudin!!!!, we form the product $\prod_{j=1}^n$, and obtain a set of equations for the (*real*) centers λ_α^n:

$$\left[e_n(\lambda_\alpha^n)\right]^N = (-)^n \prod_{m=1}^\infty \prod_{\beta=0}^{M_m} E_{nm}(\lambda_\alpha^n - \lambda_\beta^m)\,, \tag{2.7}$$

where

$$E_{nm}(\lambda) \equiv e_{|n-m|}(\lambda)\; e^2_{|n-m|+2}(\lambda)\; \cdots\; e^2_{n+m-2}(\lambda)\; e_{n+m}(\lambda)\,. \tag{2.8}$$

In obtaining this result, we use the lemmas

$$\prod_{j=1}^n e_m(\lambda_\alpha^{(n,j)}) = \prod_{l=1}^{min(n,m)} e_{n+m+1-2l}(\lambda_\alpha^n)\,, \tag{2.9}$$

$$\prod_{j=1}^n \prod_{k=1}^m e_2(\lambda_\alpha^{(n,j)} - \lambda_\beta^{(m,k)}) = E_{nm}(\lambda_\alpha^n - \lambda_\beta^m)\,. \tag{2.10}$$

Since the equations (2.7) involve only products of phases, it is useful to take the logarithm:

$$N p_n(\lambda_\alpha^n) = 2\pi J_\alpha^n + \sum_{m=1}^{\infty} \sum_{\beta=0}^{M_m} \Xi_{nm}(\lambda_\alpha^n - \lambda_\beta^m)\,, \tag{2.11}$$

where

$$p_n(\lambda) \equiv i \ln e_n(\lambda)\,, \qquad\qquad \Xi_{nm}(\lambda) \equiv i \ln E_{nm}(\lambda)\,, \tag{2.12}$$

and J_α^n are integers or half-integers constrained by

$$-J_{max}^n \le J_\alpha^n \le J_{max}^n\,. \tag{2.13}$$

Faddeev and Takhtajan have given[!!!!] a prescription for determining an explicit expression for J_{max}^n from (2.11). Any integer or half-integer in the range (2.13) is called “admissible”. We adopt the important hypothesis that the numbers $\{J_\alpha^n\}$ can be regarded as quantum numbers of the model: for every admissible set $\{J_\alpha^n\}$ (no two of which are identical), there is a unique solution $\{\lambda_\alpha^n\}$ (no two of which are identical) of Eq. (2.11). Such solutions are called “particle rapidities”.

As we shall see, it is useful to introduce (following Yang and Yang[!!!!]) the concept of “hole”. Given a set of quantum numbers $\{J_\alpha^n\}$, we define the set of numbers $\{\tilde J_\alpha^n\}$ to be the admissible values *not* in $\{J_\alpha^n\}$. We define corresponding quantities $\{\tilde\lambda_\alpha^n\}$, called “hole rapidities”, by

$$N p_n(\tilde\lambda_\alpha^n) = 2\pi \tilde J_\alpha^n + \sum_{m=1}^{\infty} \sum_{\beta=0}^{M_m} \Xi_{nm}(\tilde\lambda_\alpha^n - \lambda_\beta^m)\,. \tag{2.14}$$

For $N \to \infty$, the distributions of the numbers $\{\lambda_\alpha^n\}$ and $\{\tilde\lambda_\alpha^n\}$ along the real axis are characterized by corresponding particle and hole densities $\rho_n(\lambda)$ and $\tilde\rho_n(\lambda)$, respectively:

$$\begin{aligned} N\rho_n(\lambda) d\lambda &= \text{ number of } \lambda^n\text{'s in } d\lambda \\ N\tilde\rho_n(\lambda) d\lambda &= \text{ number of } \tilde\lambda^n\text{'s in } d\lambda\,. \end{aligned} \tag{2.15}$$

We must now reformulate the description of the model in terms of these densities.

We begin by exhibiting a constraint between the hole and particle densities. To this end, we define the function

$$h^n(\lambda) \equiv \frac{1}{2\pi} \left\{ N p_n(\lambda) - \sum_{m=1}^{\infty} \sum_{\beta=0}^{M_m} \Xi_{nm}(\lambda - \lambda_\beta^m) \right\}\,. \tag{2.16}$$

Evidently,

$$
\begin{aligned}
h^n(\lambda_\alpha^n) &= J_\alpha^n \,, \\
h^n(\tilde{\lambda}_\alpha^n) &= \tilde{J}_\alpha^n \,.
\end{aligned} \tag{2.17}
$$

We make the assumption, which is implicit in Refs. !!!! and !!!!, that $h^n(\lambda)$ is a monotonic increasing function of λ. It follows that

$$
\begin{aligned}
N\left[\rho_n(\lambda) + \tilde{\rho}_n(\lambda)\right] d\lambda = & \text{ number of } \lambda^n\text{'s and } \tilde{\lambda}^n\text{'s in } d\lambda \\
= & \text{ number of times } h^n(\lambda) \text{ ranges over } J_\alpha^n\text{'s and } \tilde{J}_\alpha^n\text{'s in } d\lambda \\
= & \, h^n(\lambda + d\lambda) - h^n(\lambda) = dh^n \,.
\end{aligned} \tag{2.18}
$$

That is,

$$
\rho_n(\lambda) + \tilde{\rho}_n(\lambda) = \frac{1}{N}\frac{dh^n}{d\lambda} \,. \tag{2.19}
$$

Making in Eq. (2.16) the following replacement of sums by integrals

$$
\frac{1}{N}\sum_{\beta=0}^{M_m}(\ \ ) \to \int_{-\infty}^{\infty}(\ \ )\rho_m(\lambda')d\lambda' \,, \tag{2.20}
$$

we see from (2.19) that

$$
\rho_n(\lambda) + \tilde{\rho}_n(\lambda) = \frac{1}{2\pi}\frac{dp_n(\lambda)}{d\lambda} - \sum_{m=1}^{\infty}\int_{-\infty}^{\infty}\frac{1}{2\pi}\frac{d\Xi_{nm}(\lambda-\lambda')}{d\lambda}\rho_m(\lambda')d\lambda' \,. \tag{2.21}
$$

This can be rewritten in the final form

$$
\tilde{\rho}_n + \sum_{m=1}^{\infty} A_{nm} * \rho_m = a_n \,, \tag{2.22}
$$

where

$$
\begin{aligned}
A_{nm}(\lambda) &\equiv \frac{1}{2\pi}\frac{d\Xi_{nm}(\lambda)}{d\lambda} + \delta(\lambda)\delta_{nm} \\
&= \delta(\lambda)\delta_{nm} + (1-\delta_{nm})\, a_{|n-m|}(\lambda) + a_{n+m}(\lambda) \\
&\qquad + 2 \sum_{l=1}^{min(n,m)-1} a_{|n-m|+2l}(\lambda) \,,
\end{aligned} \tag{2.23}
$$

and

$$
a_n(\lambda) \equiv \frac{1}{2\pi}\frac{dp_n(\lambda)}{d\lambda} = \frac{1}{2\pi}\frac{n}{\lambda^2 + \frac{n^2}{4}} \,, \tag{2.24}
$$

and $*$ denotes the convolution

$$(f*g)(\lambda) \equiv \int_{-\infty}^{\infty} d\lambda' \; f(\lambda-\lambda')g(\lambda') = (g*f)(\lambda)\,. \tag{2.25}$$

One can regard the constraint equation (2.22) as a definition of $\tilde{\rho}_n$ in terms of ρ_n.

We introduce here for future reference the "inverse" function

$$A^{-1}_{nm}(\lambda) \equiv \delta(\lambda)\delta_{nm} - s(\lambda)\left(\delta_{n,m+1} + \delta_{n,m-1}\right)\,, \tag{2.26}$$

where $s(\lambda)$ is defined by

$$s(\lambda) \equiv \frac{1}{2\,\mathrm{ch}\,\pi\lambda}\,. \tag{2.27}$$

It has the properties that

$$\sum_{n'=1}^{\infty} \left(A^{-1}_{nn'} * A_{n'm}\right)(\lambda) = \delta(\lambda)\delta_{nm}\,, \tag{2.28}$$

and

$$\sum_{m=1}^{\infty} \left(A^{-1}_{nm} * a_m\right)(\lambda) = s(\lambda)\delta_{n1}\,, \qquad \sum_{m=1}^{\infty} A^{-1}_{nm} * m = 0\,. \tag{2.29}$$

These relations can be easily derived with the help of Fourier transforms, for which we use the following conventions:

$$\hat{f}(\omega) \equiv \int_{-\infty}^{\infty} e^{i\omega\lambda}\; f(\lambda)d\lambda\,, \qquad f(\lambda) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-i\omega\lambda}\; \hat{f}(\omega)d\omega\,. \tag{2.30}$$

In particular, we note the convolution theorem

$$\int_{-\infty}^{\infty} e^{i\omega\lambda}\; (f*g)(\lambda)\; d\lambda = \hat{f}(\omega)\; \hat{g}(\omega)\,, \tag{2.31}$$

and the identities

$$\hat{a}_n(\omega) = \begin{cases} e^{-n|\omega|/2} & n>0 \\ 0 & n=0 \end{cases}\,, \qquad \hat{s}(\omega) = \frac{1}{2\,\mathrm{ch}\,\frac{\omega}{2}}\,, \tag{2.32}$$

$$\hat{A}_{nm}(\omega) = \left(\mathrm{cth}\,\frac{|\omega|}{2}\right)\left[e^{-|n-m||\omega|/2} - e^{-(n+m)|\omega|/2}\right]\,, \tag{2.33}$$

$$\hat{A}^{-1}_{nm}(\omega) = \delta_{nm} - \hat{s}(\omega)\left(\delta_{n,m+1} + \delta_{n,m-1}\right)\,. \tag{2.34}$$

We recall that the Bethe Ansatz provides the expression (2.1) for the energy eigenvalues in terms of λ's. In order to recast this expression in terms of densities, we first invoke the string hypothesis to arrive at

$$E = -\frac{1}{2} \sum_{n=1}^{\infty} \sum_{\alpha=0}^{M_n} \sum_{j=1}^{n} \frac{1}{\left(\lambda_\alpha^{(n,j)}\right)^2 + \frac{1}{4}} - H \left(\frac{N}{2} - \sum_{n=1}^{\infty} n M_n \right) . \tag{2.35}$$

We next observe that

$$\begin{aligned} \frac{1}{2} \sum_{j=1}^{n} \frac{1}{\left(\lambda_\alpha^{(n,j)}\right)^2 + \frac{1}{4}} &= \frac{i}{2} \frac{d}{d\lambda_\alpha^n} \sum_{j=1}^{n} \ln e_1(\lambda_\alpha^{(n,j)}) = \frac{i}{2} \frac{d}{d\lambda_\alpha^n} \ln \prod_{j=1}^{n} e_1(\lambda_\alpha^{(n,j)}) \\ &= \frac{i}{2} \frac{d}{d\lambda_\alpha^n} \ln e_n(\lambda_\alpha^n) = \frac{1}{2} \frac{d}{d\lambda_\alpha^n} p_n(\lambda_\alpha^n) = \pi a_n(\lambda_\alpha^n) , \end{aligned} \tag{2.36}$$

where, in passing to the second line, we have used the lemma (2.9). It follows that the energy is given by

$$\begin{aligned} E &= -\pi \sum_{n=1}^{\infty} \sum_{\alpha=0}^{M_n} a_n(\lambda_\alpha^n) - NH \left(\frac{1}{2} - \frac{1}{N} \sum_{n=1}^{\infty} n M_n \right) \\ &= -N\pi \sum_{n=1}^{\infty} \int_{-\infty}^{\infty} a_n(\lambda) \rho_n(\lambda) d\lambda - NH \left(\frac{1}{2} - \sum_{n=1}^{\infty} n \int_{-\infty}^{\infty} \rho_n(\lambda) d\lambda \right) . \end{aligned} \tag{2.37}$$

Given a set of particle densities $\{\rho_n\}$, this expression determines an energy level of the system. Notice that this expression does not depend on the hole densities $\tilde{\rho}_n$.

As an illustration of this formalism, let us briefly consider the ground state of the system in zero field ($H = 0$). We assume that for this state, there are no holes. That is,

$$\tilde{\rho}_n = 0 . \tag{2.38}$$

(We shall prove this later from the TBA equations.) It follows from the constraint (2.22) that

$$\sum_{m=1}^{\infty} A_{nm} * \rho_m = a_n . \tag{2.39}$$

Thus, the particle densities are given by

$$\rho_n = \sum_{m=1}^{\infty} A_{nm}^{-1} * a_m = s \delta_{n1} , \tag{2.40}$$

where $s(\lambda)$ is given by (2.27). That is, the antiferromagnetic ground state is described by strings of length 1 (i.e., real solutions of the BA equations). From Eq. (2.37), we conclude that the energy per site for the ground state is

$$e_0 = \frac{E_0}{N} = -\pi \int_{-\infty}^{\infty} a_1(\lambda) s(\lambda) d\lambda = -\ln 2 \,, \tag{2.41}$$

which is the well-known result of Hulthen[!!!!].

This example raises two important questions:
(i) how to establish the result (2.38) that the ground state has no holes?
(ii) how to study low-lying excitations?
An answer to both questions is to consider the system at temperature $T \ge 0$. The equilibrium state at $T = 0$ is the ground state; and the equilibrium state at low but nonzero temperature provides information about the low-lying excitations.

We now argue heuristically, following Refs. !!!!, !!!! and !!!!, that the equilibrium state at temperature T is described by certain equilibrium densities ρ_n^{eq} and $\tilde\rho_n^{eq}$. We begin by observing that the partition function is given by

$$Z = \mathrm{tr}\, e^{-\mathcal{H}/T} = \sum_{eigenstates} e^{-E/T} = \sum_{\rho, \tilde\rho} \delta \left[\chi(\rho, \tilde\rho) \right] \; W[\rho, \tilde\rho] \; e^{-E[\rho]/T} \,, \tag{2.42}$$

where the delta function enforces the constraint

$$\chi(\rho, \tilde\rho) = 0 \,, \tag{2.43}$$

which represents the constraint (2.22), and $W[\rho, \tilde\rho]$ is equal to the number of states corresponding to given densities ρ and $\tilde\rho$. Introducing the entropy

$$S = \ln W \,, \tag{2.44}$$

and using the fact that the free energy is given by

$$F = E - TS \,, \tag{2.45}$$

we see that

$$Z = \sum_{\rho, \tilde\rho} \delta \left[\chi(\rho, \tilde\rho) \right] \; e^{-(E[\rho] - TS[\rho, \tilde\rho])/T} = \sum_{\rho, \tilde\rho} \delta \left[\chi(\rho, \tilde\rho) \right] \; e^{-F[\rho, \tilde\rho]/T} \,. \tag{2.46}$$

Using the saddle-point approximation (for $M\,, N \to \infty$ with $M/N =$ constant), we conclude that

$$Z = e^{-F[\rho_{eq}, \tilde\rho_{eq}]/T} \,, \tag{2.47}$$

where the equilibrium densities are determined by the condition

$$\delta F\Big|_{\rho=\rho_{eq}\,,\tilde{\rho}=\tilde{\rho}_{eq}} = 0\,, \tag{2.48}$$

subject to the constraint (2.43).

In order to compute the entropy (2.44), we observe (again, following Yang and Yang!!!!) that

$$\begin{aligned} dS_n &= \ln\left\{\text{number of states (strings of length } n) \text{ in } d\lambda\right\} \\ &= \ln\left\{\text{number of ways of choosing } \lambda^n\text{'s in } d\lambda\right\} \\ &= \ln\left\{\frac{[N(\rho_n+\tilde{\rho}_n)d\lambda]!}{(N\rho_n d\lambda)!\ (N\tilde{\rho}_n d\lambda)!}\right\} \\ &\approx N\left\{(\rho_n+\tilde{\rho}_n)\ln(\rho_n+\tilde{\rho}_n) - \rho_n\ln\rho_n - \tilde{\rho}_n\ln\tilde{\rho}_n\right\} d\lambda\,, \end{aligned} \tag{2.49}$$

where, in passing to the last line, we have used Stirling's approximation. We conclude that the entropy is given by

$$S = \sum_{n=1}^{\infty}\int_{-\infty}^{\infty} dS_n = N\sum_{n=1}^{\infty}\int_{-\infty}^{\infty}\left\{(\rho_n+\tilde{\rho}_n)\ln(\rho_n+\tilde{\rho}_n) - \rho_n\ln\rho_n - \tilde{\rho}_n\ln\tilde{\rho}_n\right\} d\lambda\,. \tag{2.50}$$

The hole concept was introduced precisely for calculating the entropy.

The free energy F of the Heisenberg ring is given by (2.45), with the energy E given by (2.37) and the entropy S given by (2.50). The condition $\delta F = 0$ subject to the constraint (2.22) yields the thermodynamic Bethe Ansatz (TBA) equations

$$T\ln\left(1+e^{\epsilon_n/T}\right) = \sum_{m=1}^{\infty} A_{nm} * T\ln\left(1+e^{-\epsilon_m/T}\right) - \pi a_n + nH\,, \tag{2.51}$$

where the functions $\epsilon_n(\lambda)$ are defined by

$$\epsilon_n(\lambda) = T\ln\left(\frac{\tilde{\rho}_n^{eq}(\lambda)}{\rho_n^{eq}(\lambda)}\right)\,. \tag{2.52}$$

The TBA equations are an infinite set of coupled, nonlinear integral equations, which we shall assume to have a unique solution $\{\epsilon_n(\lambda)\}$. It follows that $\{\epsilon_n(\lambda)\}$ are even functions of λ,

$$\epsilon_n(-\lambda) = \epsilon_n(\lambda)\,. \tag{2.53}$$

Having solved for these functions, one can then use the constraint equations (2.22) to determine the equilibrium densities $\{\rho_n^{eq}(\lambda)\}$ and $\{\tilde{\rho}_n^{eq}(\lambda)\}$.

The free energy per site at equilibrium is given by

$$\frac{F}{N} = -T \sum_{n=1}^{\infty} \int_{-\infty}^{\infty} d\lambda\, a_n(\lambda) \ln\left(1 + e^{-\epsilon_n(\lambda)/T}\right) - \frac{1}{2} H \,. \tag{2.54}$$

This result is obtained by using the constraint equations (2.22) to eliminate $\tilde{\rho}_n$ from the expression for F/N, and then noting that the coefficient of ρ_n vanishes by virtue of the TBA equations. Alternatively, by eliminating $\tilde{\rho}_n$, one can show that

$$\frac{F}{N} = e_0 - T \int_{-\infty}^{\infty} d\lambda\, s(\lambda) \ln\left[1 + e^{\epsilon_1(\lambda)/T}\right] , \tag{2.55}$$

where e_0 is given by (2.41). This expression for the equilibrium free energy is particularly useful, since it depends on only *one* of the $\epsilon_n(\lambda)$'s.

3. Thermodynamics for small T and H

In this section, we shall solve the TBA equations (2.51) for $\epsilon_1(\lambda)$ for small values of T and H, and evaluate the expression (2.55) for the free energy.

As we have seen, the TBA equations are an infinite set of coupled equations. A significant simplification occurs for $T \rightarrow 0$: namely, the equation for $\epsilon_1(\lambda)$ becomes decoupled from the other equations. In order to see this, we first cast the TBA equations in the form given by Takahashi[!!!!]:

$$\begin{aligned} \epsilon_1 &= -\pi a_1 + H + a_2 * T \ln\left(1 + e^{-\epsilon_1/T}\right) \\ &\qquad + (a_0 + a_2) * \sum_{m=1}^{\infty} a_m * T \ln\left(1 + e^{-\epsilon_{m+1}/T}\right) , \end{aligned} \tag{3.1}$$

$$\begin{aligned} \epsilon_n &= H + a_1 * T \ln\left(1 + e^{\epsilon_{n-1}/T}\right) + a_2 * T \ln\left(1 + e^{-\epsilon_n/T}\right) \\ &\qquad + (a_0 + a_2) * \sum_{m=1}^{\infty} a_m * T \ln\left(1 + e^{-\epsilon_{m+n}/T}\right) , \qquad n \geq 2 \,, \end{aligned} \tag{3.2}$$

where $a_0(\lambda) = \delta(\lambda)$. To obtain Eq. (3.1), we start by writing the $n = 1$ TBA equation using the explicit form of A_{1m} as given in (2.23). We then rearrange the terms and use the identities

$$a_n * a_m = a_{n+m} \,. \tag{3.3}$$

To obtain the equation for ϵ_2, we use the additional identity

$$a_n * H = H \tag{3.4}$$

to write the driving term $-\pi a_2 + 2H$ of the $n = 2$ TBA equation as $a_1 * (-\pi a_1 + H) + H$, and we then use Eq. (3.1) to eliminate the terms in parenthesis. The other equations are obtained by following the same strategy.

From this form of the equations, we conclude that

$$\epsilon_n(\lambda) \geq 0 \qquad \text{for } n \geq 2 \, . \tag{3.5}$$

This positivity property will play an important role in the arguments that follow.*

Consider now Eq. (3.1). The positivity property (3.5) implies that $\exp(-\epsilon_{m+1}/T)$ goes to zero exponentially as $T \to 0$ for $m \geq 1$ and can therefore be neglected. This is the reason for the decoupling of equations mentioned above. On the other hand, $\epsilon_1(\lambda)$ can have either sign. Defining $\varepsilon(\lambda)$ to be the $T \to 0$ limit of $\epsilon_1(\lambda)$, we see that

$$\lim_{T \to 0} \, T \ln \left(1 + e^{\pm \epsilon_1 / T} \right) = \pm \varepsilon^{\pm} \, , \tag{3.6}$$

where we use the standard notation

$$\varepsilon^{-} \equiv \frac{1}{2} \left(\varepsilon - |\varepsilon| \right) \, , \qquad \qquad \varepsilon^{+} \equiv \varepsilon - \varepsilon^{-} \, . \tag{3.7}$$

It follows from (3.1) that

$$\varepsilon = -\pi a_1 + H - a_2 * \varepsilon^{-} \, . \tag{3.8}$$

It will be convenient for subsequent analysis to work with the following equivalent equation, which does not involve ε^{-}:

$$\varepsilon = \frac{1}{2} H - \pi s + h * \varepsilon^{+} \, , \tag{3.9}$$

where $s(\lambda)$ is defined in (2.27), and $h(\lambda)$ is defined by

$$h = s * a_1 \, . \tag{3.10}$$

In order to obtain (3.9), we substitute $\varepsilon^{-} = \varepsilon - \varepsilon^{+}$ into (3.8); and we then solve for ε in terms of ε^{+} with the help of Fourier transforms. We observe for future reference

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* An alternative way of demonstrating this positivity property relies on the "inverted" TBA equations, which are obtained by forming the convolution of the TBA equations with A^{-1}_{nm}. However, these equations must be supplemented with a condition on ϵ_n for $n \to \infty$.

that by a similar procedure, (3.1) can be recast (after neglecting the infinite sum, but before taking the $T \to 0$ limit of ϵ_1) as follows:

$$\epsilon_1 = \frac{1}{2}H - \pi s + h * T \ln\left(1 + e^{\epsilon_1/T}\right) . \tag{3.11}$$

Evidently, the $T \to 0$ limit of this equation gives (3.9).

We have obtained the linear integral equation (3.9) for ε. Of central importance in obtaining this result was the positivity property (3.5). We shall now show that Eq. (3.9) can be solved, and that it has a unique solution. We shall also establish certain properties of the solution, which will turn out to be crucial for formulating the linear integral equation obeyed by the leading correction to this lowest-order result.

We first briefly consider the case $H = 0$, which corresponds to the ground (vacuum) state. Since $s(\lambda)$ is positive for all λ, Eq. (3.9) has the solution

$$\varepsilon(\lambda) = -\pi s(\lambda) = -\frac{\pi}{2\,\mathrm{ch}\,\pi\lambda} . \tag{3.12}$$

From the definition (2.52), the constraint equation (2.22), and the positivity property (3.5), it follows that the ground-state densities of holes and particles are precisely those anticipated in the previous section. (See Eqs. (2.38) and (2.40), respectively.)

We turn now to the case $H \neq 0$. We observe, following Yang and Yang and Takahashi, that Eq. (3.9) can be solved by iteration. Indeed, set

$$\varepsilon_{(0)}(\lambda) = \frac{1}{2}H - \pi s(\lambda) , \tag{3.13}$$

$$\varepsilon_{(n)}(\lambda) = \frac{1}{2}H - \pi s(\lambda) + \left(h * \varepsilon^{+}_{(n-1)}\right)(\lambda) , \qquad n \geq 1 . \tag{3.14}$$

If the sequence $\{\varepsilon_{(0)}(\lambda)\, , \varepsilon_{(1)}(\lambda)\, , \cdots\}$ has a limit

$$\lim_{n\to\infty} \varepsilon_{(n)}(\lambda) = \varepsilon(\lambda) , \tag{3.15}$$

then this limit satisfies Eq. (3.9). In order to show that this sequence is convergent, we prove that it is monotonically increasing (i.e., $\varepsilon_{(n)}(\lambda) > \varepsilon_{(n-1)}(\lambda)$) and that it is bounded from above. To demonstrate that the sequence is monotonically increasing, we proceed by induction, using the fact that $h(\lambda)$ is positive for all λ, and that

$$\varepsilon_{(n)} = \varepsilon_{(n-1)} + h * \left(\varepsilon^{+}_{(n-1)} - \varepsilon^{+}_{(n-2)}\right) , \qquad n \geq 2 . \tag{3.16}$$

To show that the sequence is bounded from above, we cast the relation (3.14) in the form

$$\varepsilon_{(n)} = \varepsilon_{(0)} + h * \varepsilon^{+}_{(0)} + \cdots + h * \cdots * h * \varepsilon^{+}_{(0)} \,, \tag{3.17}$$

where in the last term the factor h appears n times. From (3.13), we see that $\varepsilon_{(0)}(\lambda) < H/2$. It follows that

$$h * \cdots * h * \varepsilon^{+}_{(0)}(\lambda) < \left(\frac{1}{2}\right)^{n} \frac{H}{2} \,, \tag{3.18}$$

and therefore

$$\varepsilon_{(n)}(\lambda) < \frac{2^{n+1} - 1}{2^{n+1}} H \,. \tag{3.19}$$

We conclude that

$$\varepsilon_{(n)}(\lambda) < H \tag{3.20}$$

for any n, and so the sequence is bounded from above. This completes the proof that the iteration procedure (3.13), (3.14) gives a solution of Eq. (3.9).

From this iterative solution, we can understand the general behavior of $\varepsilon(\lambda)$ as a function of λ. For $\lambda > 0$, this function is monotonically increasing. Indeed, following again Refs. !!!! and !!!!, we prove the monotonicity of $\varepsilon_{(n)}(\lambda)$ by induction. From (3.13), we determine that $\varepsilon'_{(0)}(\lambda) > 0$ for $\lambda > 0$. Differentiating (3.14) with respect to λ, we obtain

$$\varepsilon'_{(n)}(\lambda) = \varepsilon'_{(0)}(\lambda) + \int_{-\infty}^{\infty} h(\lambda - \zeta)\ \varepsilon^{+\prime}_{(n-1)}(\zeta)\ d\zeta \tag{3.21}$$

$$= \varepsilon'_{(0)}(\lambda) + \int_{0}^{\infty} \left[h(\lambda - \zeta) - h(\lambda + \zeta)\right]\ \varepsilon^{+\prime}_{(n-1)}(\zeta)\ d\zeta \,. \tag{3.22}$$

Since the function $h(\lambda)$ is even and monotonically decreasing for $\lambda > 0$, the expression inside the brackets in Eq. (3.22) is positive. Therefore, if $\varepsilon'_{(n-1)}(\lambda) > 0$ for $\lambda > 0$, then $\varepsilon'_{(n)}(\lambda) > 0$ for $\lambda > 0$. This concludes the proof that $\varepsilon_{(n)}(\lambda)$ (and hence $\varepsilon(\lambda)$) is a monotonic increasing function of λ, for $\lambda > 0$.

On the other hand, we have seen that $\varepsilon(\lambda)$ is bounded from above. Therefore, the function $\varepsilon(\lambda)$ has the following general behavior:

figure available on request

In particular, $\varepsilon(\lambda)$ has only one zero for $\lambda > 0$,

$$\varepsilon(\alpha) = 0 \,. \tag{3.23}$$

Hence, $\varepsilon(\lambda) < 0$ for λ in the interval $(0\,,\alpha)$, and $\varepsilon(\lambda) > 0$ for λ in the interval $(\alpha\,,\infty)$.

Observe that Eq. (3.9) is temperature-independent. Using the same approximations in the expression (2.55) for the free energy this too will be temperature-independent. As emphasized by Johnson and McCoy[!!!!], to find the leading order temperature dependence one must compute the leading correction to the solution $\epsilon_1 = \varepsilon$ of the linearized equation (3.9). In order to obtain this correction, we make the substitution

$$\epsilon_1(\lambda) = \varepsilon(\lambda) + \eta(\lambda) \tag{3.24}$$

in (3.11) and expand to leading order in η. Since ε is a solution of the linearized equation (3.9), we shall find an inhomogeneous term in the resulting equation for η. Indeed, we have that

$$\eta = h * \left\{ T \ln \left[1 + e^{(\varepsilon+\eta)/T} \right] - \varepsilon^+ \right\} . \tag{3.25}$$

Because $\varepsilon(\lambda)$ is an even function of λ with a single zero, at $\lambda = \alpha$, for positive λ, we see that

$$\begin{aligned} \eta(\lambda) = & \left(\int_{-\infty}^{-\alpha} + \int_{\alpha}^{\infty} \right) d\lambda'\ h(\lambda-\lambda') \left\{ T \ln \left[1 + e^{\left(\varepsilon(\lambda')+\eta(\lambda')\right)/T} \right] - \varepsilon(\lambda') \right\} \\ & + \int_{-\alpha}^{\alpha} d\lambda'\ h(\lambda-\lambda')\ T \ln \left[1 + e^{\left(\varepsilon(\lambda')+\eta(\lambda')\right)/T} \right] \\ \approx & \left(\int_{-\infty}^{-\alpha} + \int_{\alpha}^{\infty} \right) d\lambda'\ h(\lambda-\lambda')\ \eta(\lambda') + E_h(\lambda) \end{aligned} \tag{3.26}$$

where the inhomogeneous term $E_h(\lambda)$ is given by

$$E_h = h * T \ln \left(1 + e^{-|\varepsilon|/T} \right) . \tag{3.27}$$

For $T \to 0$, the major contribution to the integral comes from the regions near the zeros of ε, so we expand $\varepsilon(\lambda)$ about $\lambda = \alpha$,

$$\varepsilon(\lambda) = t\,(\lambda-\alpha) + O\left((\lambda-\alpha)^2\right) , \qquad\qquad t \equiv \left.\frac{d\varepsilon}{d\lambda}\right|_{\lambda=\alpha} . \tag{3.28}$$

One then finds that the leading T- dependence of E_h is

$$\begin{aligned} E_h(\lambda) &= \frac{2T^2}{t} \left[h(\lambda-\alpha) + h(\lambda+\alpha) \right] \int_0^\infty du\ \ln\left(1+e^{-u}\right) \\ &= \frac{\pi^2 T^2}{6t} \left[h(\lambda-\alpha) + h(\lambda+\alpha) \right] . \end{aligned} \tag{3.29}$$

Thus, we obtain the following linear, but nonlocal, equation for η,*

$$\eta(\lambda) = \left(\int_{-\infty}^{-\alpha} + \int_{\alpha}^{\infty}\right) d\lambda'\; h(\lambda-\lambda')\;\eta(\lambda') + \frac{\pi^2 T^2}{6t}\left[h(\lambda-\alpha) + h(\lambda+\alpha)\right]\,. \quad (3.30)$$

This equation for η and that of (3.9) for ε complete our results for the T - expansion of ϵ_1. We turn now to the expansion for small values of H, by which from Eqs. (3.9) and (3.30) we shall generate a pair of integral equations of the Wiener-Hopf type. (For a detailed exposition of Wiener-Hopf equations, see Ref. !!!!.)

For $H \to 0$, we see from the solution of the zeroth-order equation (3.13) that the function $\varepsilon(\lambda)$ has a zero for $\lambda = \alpha = O(\ln H)$. Assuming an expansion in powers of $(\ln H)^{-1}$, we conclude that

$$\alpha = -\frac{1}{\pi}\left[\ln\left(\frac{1}{2\pi}H\right) + \ln\kappa + O\left(\frac{1}{\ln H}\right)\right]\,, \quad (3.31)$$

where the constant κ (which is independent of H) has still to be determined.

It will prove convenient to work with the functions

$$S(\lambda) = \begin{cases} e^{\pi\alpha}\;\kappa\;\varepsilon(\lambda+\alpha) & \lambda > 0 \\ 0 & \lambda < 0 \end{cases}\,, \quad (3.32)$$

and

$$T(\lambda) = \begin{cases} \frac{6e^{-\pi\alpha}}{\pi^2 T^2 \kappa}\eta(\lambda+\alpha) & \lambda > 0 \\ 0 & \lambda < 0 \end{cases}\,, \quad (3.33)$$

instead of the functions $\varepsilon(\lambda)$ and $\eta(\lambda)$. The factors $e^{\pi\alpha}$ and $e^{-\pi\alpha}/T^2$ in (3.32) and (3.33), respectively, are chosen such that the driving terms in the equations for $S(\lambda)$ and $T(\lambda)$ have a nonvanishing limit as $T \to 0$ and $H \to 0$.

We return now to Eq. (3.9). Following Refs. !!!! and !!!!, we write the limits of integration explicitly, keeping in mind that $\varepsilon(\lambda) > 0$ for $-\infty < \lambda < -\alpha$ and for $\alpha < \lambda < \infty$; and we shift the integration variables so that they run from 0 to ∞. Since $h\left(\lambda + 2\alpha\right)$ vanishes as $H \to 0$ $(\alpha \to \infty)$ for finite λ, we see that the $H \to 0$ limit of the equation for $S(\lambda)$ is

$$S(\lambda) = \pi\left(1 - \kappa e^{-\pi\lambda}\right) + \int_0^{\infty} d\lambda'\; h(\lambda-\lambda')\; S(\lambda')\,, \qquad \lambda \geq 0\,. \quad (3.34)$$

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* While Johnson and McCoy obtain this equation from the "inverted" TBA equations, we obtain it directly from the TBA equations.

Similarly, from (3.30), we see that the $H \to 0$ limit of the equation for $T(\lambda)$ is

$$T(\lambda) = \frac{h(\lambda)}{S'(0)} + \int_0^\infty d\lambda' \ h(\lambda - \lambda') \ T(\lambda') \,, \qquad \lambda \geq 0 \,, \tag{3.35}$$

where

$$S'(0) \equiv \frac{d}{d\lambda} S(\lambda)\Big|_{\lambda=0+} = e^{\pi\alpha} \kappa \ t \,. \tag{3.36}$$

These equations can be written in the standard Wiener-Hopf form

$$\begin{aligned} S(\lambda) &= f_S(\lambda) + b_S(\lambda) + \int_{-\infty}^\infty d\lambda' \ h(\lambda - \lambda') \ S(\lambda') \,, \\ T(\lambda) &= f_T(\lambda) + b_T(\lambda) + \int_{-\infty}^\infty d\lambda' \ h(\lambda - \lambda') \ T(\lambda') \,, \\ & \qquad\qquad - \infty < \lambda < \infty \,, \end{aligned} \tag{3.37}$$

where

$$f_S(\lambda) = \begin{cases} \pi \left(1 - \kappa e^{-\pi\lambda} \right) & \lambda > 0 \\ 0 & \lambda < 0 \end{cases} \,, \tag{3.38}$$

$$b_S(\lambda) = \begin{cases} 0 & \lambda > 0 \\ - \int_{-\infty}^\infty d\lambda' \ h(\lambda - \lambda') \ S(\lambda') & \lambda < 0 \end{cases} \,, \tag{3.39}$$

and similarly

$$f_T(\lambda) = \begin{cases} \frac{h(\lambda)}{S'(0)} & \lambda > 0 \\ 0 & \lambda < 0 \end{cases} \,, \tag{3.40}$$

$$b_T(\lambda) = \begin{cases} 0 & \lambda > 0 \\ - \int_{-\infty}^\infty d\lambda' \ h(\lambda - \lambda') \ T(\lambda') & \lambda < 0 \end{cases} \,. \tag{3.41}$$

We shall solve these equations by Fourier transform. Since $S(\lambda)$ and $T(\lambda)$ vanish for $\lambda < 0$, the Fourier transforms $\hat{S}(\omega)$ and $\hat{T}(\omega)$ are analytic in the upper-half-plane Im $\omega \geq 0$, which we denote by Π_+. Observe that

$$S(0) = \frac{2}{2\pi} \int_{-\infty}^\infty d\omega \ \hat{S}(\omega) \,, \tag{3.42}$$

where the factor 2 in the numerator is due to the discontinuity of $S(\lambda)$ at $\lambda = 0$. Evidently, the contour integral of $\hat{S}(\omega)$ along a closed contour in Π_+ is zero. By explicitly evaluating the contribution of the semi-circle at infinity, we obtain

$$\int_{-\infty}^\infty d\omega \ \hat{S}(\omega) = - \int_{semi-circle} d\omega \ \hat{S}(\omega) = -i\pi \lim_{|\omega| \to \infty} \ \omega \hat{S}(\omega) \,, \tag{3.43}$$

where the limit is taken in Π_+. On the other hand, $S(0) = 0$, as follows from $\varepsilon(\alpha) = 0$. Therefore,

$$S(0) = -i \lim_{|\omega|\to\infty} \omega \hat{S}(\omega) = 0\,. \tag{3.44}$$

Similarly,

$$S'(0) = \frac{d}{d\lambda} S(\lambda)\Big|_{\lambda=0+} = - \lim_{|\omega|\to\infty} \omega^2 \hat{S}(\omega)\,. \tag{3.45}$$

In deriving this result, we must again include a factor 2 due to the discontinuity (here, of $S'(\lambda)$) at $\lambda = 0$.

The Wiener-Hopf equations in Fourier space are

$$\hat{S}(\omega) = \hat{f}_S(\omega) + \hat{b}_S(\omega) + \hat{h}(\omega)\ \hat{S}(\omega)\,, \tag{3.46}$$
$$\hat{T}(\omega) = \hat{f}_T(\omega) + \hat{b}_T(\omega) + \hat{h}(\omega)\ \hat{T}(\omega)\,. \tag{3.47}$$

Since $\hat{h}(-\omega) = \hat{h}(\omega)$ and $1 - \hat{h}(\omega) \neq 0$ for $-\infty < \omega < \infty$, there exists!!!! a unique factorization

$$\Big(1 - \hat{h}(\omega)\Big)^{-1} = G_+(\omega)\ G_-(\omega)\,, \qquad -\infty < \omega < \infty\,, \tag{3.48}$$

where $G_+(\omega)$ and $G_-(\omega)$ are functions that are analytic and nonvanishing in the half-planes Π_+ and Π_-, respectively, and are normalized by the condition

$$G_+(\infty) = G_-(\infty) = 1\,. \tag{3.49}$$

Moreover, the fact $h(-\lambda) = h(\lambda)$ implies that (for ω in Π_-)

$$G_-(\omega) = G_+(-\omega)\,. \tag{3.50}$$

As we shall see, explicit expressions for G_+ and G_- are not needed to compute the free energy to the order in which we work. A similar phenomenon occurs in the Wiener-Hopf calculations of Yang and Yang!!!!.

These properties will be used to solve the Wiener-Hopf equations (3.46) and (3.47), to which we now turn. Using the factorization (3.48), the equation (3.46) for $\hat{S}$ can be rewritten as

$$G_+^{-1}\ \hat{S} = G_- \left(\hat{f}_S + \hat{b}_S\right)\,. \tag{3.51}$$

Observe that the left hand side is analytic and bounded in Π_+, whereas $G_-\hat{b}_S$ is analytic and bounded in Π_-. The term $G_-\hat{f}_S$ has a decomposition as

$$G_-\hat{f}_S = P_-\left(G_-\hat{f}_S\right) + P_+\left(G_-\hat{f}_S\right)\,, \tag{3.52}$$

where $P_\pm\left(G_-\hat{f}_S\right)$ is analytic in $\Pi_\pm$. This decomposition is uniquely specified by the requirement $P_\pm\left(G_-\hat{f}_S\right) \to 0$ for $\omega \to \infty$ in $\Pi_\pm$. Taking the P_+ projection of (3.51), we have that

$$\hat{S} = G_+ \; P_+\left(G_-\hat{f}_S\right) . \tag{3.53}$$

From (3.38) we compute that

$$\hat{f}_S(\omega) = \pi i \left(\frac{1}{\omega + i\epsilon} - \frac{\kappa}{\omega + \pi i}\right) , \tag{3.54}$$

where one is to take $\epsilon \to 0$ at the end. The decomposition (3.52) of $G_-\hat{f}_S$ is then found by subtracting the residues of $\hat{f}_S$, i.e.,

$$\begin{aligned} G_-(\omega)\hat{f}_S(\omega) =& \pi i \left\{\frac{1}{\omega + i\epsilon}\left(G_-(\omega) - G_-(-i\epsilon)\right) - \frac{\kappa}{\omega + \pi i}\left(G_-(\omega) - G_-(-\pi i)\right)\right\} \\ &+ \pi i \left\{\frac{1}{\omega + i\epsilon} G_-(-i\epsilon) - \frac{\kappa}{\omega + \pi i} G_-(-\pi i)\right\} . \end{aligned} \tag{3.55}$$

Hence,

$$\hat{S}(\omega) = \frac{\pi i}{\omega + i\epsilon} G_+(\omega) G_-(0) - \frac{\pi i \kappa}{\omega + \pi i} G_+(\omega) G_-(-\pi i) . \tag{3.56}$$

The boundary condition (3.44) implies that the parameter κ is given by

$$\kappa = G_-(-\pi i)^{-1} \; G_-(0) . \tag{3.57}$$

Using this result we conclude that $\hat{S}(\omega)$ is given by

$$\hat{S}(\omega) = \pi i \left(\frac{1}{\omega + i\epsilon} - \frac{1}{\omega + \pi i}\right) G_+(\omega) G_-(0) . \tag{3.58}$$

From Eq. (3.45) and the fact that $G_+(\omega) \to 1$ as $|\omega| \to \infty$ in Π_+, we find that

$$S'(0) = \pi^2 G_-(0) . \tag{3.59}$$

We turn now to the equation (3.47) for $\hat{T}(\omega)$. Proceeding as before, we use the factorization (3.48) to arrive at the formal solution

$$\hat{T} = G_+ \; P_+\left(G_-\hat{f}_T\right) \tag{3.60}$$

(cf. Eq. (3.53)). The explicit calculation of $\hat{f}_T$ is difficult, but can be avoided by the following trick. Consider the functions $f(\lambda)$ defined as

$$f(\lambda) = \frac{h(\lambda)}{S'(0)} \,, \tag{3.61}$$

where λ ranges over the entire real line. From Eq. (3.40), it is evident that

$$f_T(\lambda) = f_+(\lambda) \,, \tag{3.62}$$

where

$$f_+(\lambda) \equiv \left\{ \begin{array}{cc} f(\lambda) & \lambda > 0 \\ 0 & \lambda < 0 \end{array} \right. , \qquad f_-(\lambda) \equiv \left\{ \begin{array}{cc} 0 & \lambda > 0 \\ f(\lambda) & \lambda < 0 \end{array} \right. , \qquad f = f_+ + f_- \,. \tag{3.63}$$

The Fourier transform of $f(\lambda)$ is readily computed:

$$\hat{f}(\omega) = \frac{\hat{h}(\omega)}{S'(0)} \,. \tag{3.64}$$

From the factorization (3.48), it follows that

$$\hat{f}_+ + \hat{f}_- = \left(1 - G_-^{-1} G_+^{-1}\right) \frac{1}{S'(0)} \,. \tag{3.65}$$

After multiplying both sides of this equation by G_-, we see that the P_+ projection of $G_- \hat{f}_+$ is given by

$$P_+ \left(G_- \hat{f}_+ \right) = \alpha - \frac{G_+^{-1}}{S'(0)} \,, \tag{3.66}$$

where α is a constant. Requiring the right hand side to vanish for $|\omega| \to \infty$ in Π_+ determines this constant to be

$$\alpha = \frac{1}{S'(0)} \,. \tag{3.67}$$

We conclude from (3.60) that $\hat{T}(\omega)$ is given by

$$\hat{T}(\omega) = \left(G_+(\omega) - 1 \right) \frac{1}{S'(0)} \,, \tag{3.68}$$

where $S'(0)$ is given by (3.59).

To summarize: we have made the expansion (3.24) of $\epsilon_1(\lambda)$, and we have changed in Eqs. (3.32), (3.33) from the variables $\varepsilon(\lambda)$, $\eta(\lambda)$ to the variables $S(\lambda)$, $T(\lambda)$, respectively. Using Wiener-Hopf methods, we have determined in Eqs. (3.58), (3.68) the corresponding Fourier transforms $\hat{S}(\omega)$, $\hat{T}(\omega)$ in the limits $T \to 0$ and $H \to 0$. These expressions involve $G_+(\omega)$ and $G_-(\omega)$, which appear in the factorization (3.48). We shall now use these results to calculate the free energy.

Substituting the expansion (3.24) of $\epsilon_1(\lambda)$ into the expression (2.55) for the free energy (keeping in mind the discussion immediately following (3.24)), we obtain

$$\frac{F}{N} = e_0 - \frac{\pi^2 T^2 s(\alpha)}{3t} - 2\int_\alpha^\infty d\lambda\ s(\lambda)\left[\varepsilon(\lambda) + \eta(\lambda)\right] , \tag{3.69}$$

where the ground state energy per site e_0 is given by (2.41).

We aim for a double expansion of F/N to quadratic order in both T and H. To this end, we rewrite (3.69) in terms of $S(\lambda)$ and $T(\lambda)$. Consider first the T^2 term. For $H \to 0$, we can make the approximation

$$s(\alpha) = e^{-\pi\alpha} , \tag{3.70}$$

and hence (remembering (3.36)) this term becomes

$$-\frac{\pi^2 T^2 \kappa}{3 S'(0)} . \tag{3.71}$$

We next manipulate the integral in the last term as follows:

$$\int_\alpha^\infty d\lambda\ s(\lambda)\left[\varepsilon(\lambda) + \eta(\lambda)\right] = \int_0^\infty d\lambda\ s(\lambda+\alpha)\left[\frac{e^{-\pi\alpha}}{\kappa} S(\lambda) + \frac{\pi^2 T^2 \kappa}{6 e^{-\pi\alpha}} T(\lambda)\right] . \tag{3.72}$$

Taking the $\alpha \to \infty$ limit of this expression, we arrive at the following expression for F/N,

$$\frac{F}{N} = e_0 - \frac{H^2 \kappa}{2\pi^2}\int_0^\infty d\lambda\ e^{-\pi\lambda} S(\lambda) - \frac{\pi^2 T^2 \kappa}{3}\left[\int_0^\infty d\lambda\ e^{-\pi\lambda} T(\lambda) + \frac{1}{S'(0)}\right] . \tag{3.73}$$

Writing the functions $S(\lambda)$ and $T(\lambda)$ as the Fourier transforms of $\hat{S}(\omega)$ and $\hat{T}(\omega)$, respectively, and then performing both the λ and ω integrals, we obtain

$$\frac{F}{N} = e_0 - \frac{H^2}{2\pi^2} A - \frac{\pi^2 T^2}{3} B , \tag{3.74}$$

with

$$A = \kappa \hat{S}(\pi i) , \qquad B = \kappa\left[\hat{T}(\pi i) + \frac{1}{S'(0)}\right] . \tag{3.75}$$

The parameter κ is given in Eq. (3.57); and using the property (3.50), this parameter can be reexpressed as

$$\kappa = G_{+}(0) G_{+}(\pi i)^{-1} \,. \tag{3.76}$$

We consider now A. Evaluating $\hat{S}(\pi i)$ using the expression (3.58), we obtain

$$A = \frac{1}{2} G_{+}(0) G_{-}(0) \,. \tag{3.77}$$

Recalling the factorization equation (3.48) and the fact that

$$\hat{h}(\omega) = \hat{s}(\omega)\ \hat{a}_1(\omega) \,, \tag{3.78}$$

we conclude that

$$A = \frac{1}{2} \left(1 - \hat{h}(0)\right)^{-1} = 1 \,. \tag{3.79}$$

There remains to compute B. Evaluating $\hat{T}(\pi i)$ using the expression (3.68), we obtain (after a crucial cancelation)

$$B = \frac{G_{+}(0)}{S'(0)} \,. \tag{3.80}$$

Recalling the expression (3.59) for $S'(0)$ and using again the property (3.50), we see that

$$B = \frac{1}{\pi^2} \,. \tag{3.81}$$

The expression for the free energy per site is therefore

$$\frac{F}{N} = e_0 - \frac{1}{2\pi^2} H^2 - \frac{1}{3} T^2 \,. \tag{3.82}$$

As foreseen above, this result was obtained without using explicit expressions for G_{+} and G_{-}. It follows that the magnetic susceptibility and specific heat, to lowest order, are given by

$$\begin{aligned} \chi &= -\frac{\partial^2}{\partial H^2} \left(\frac{F}{N}\right)\Big|_{T} = \frac{1}{\pi^2} \,, \\ C_H &= -T \frac{\partial^2}{\partial T^2} \left(\frac{F}{N}\right)\Big|_{H} = \frac{2}{3} T \,. \end{aligned} \tag{3.83}$$

For a critical chain, the free energy per site is given by!!!!

$$\frac{F}{N} = e_0 - \frac{\pi c}{6 v_s} T^2 + \cdots \,, \tag{3.84}$$

where c is the central charge and v_s is the velocity of sound. For the antiferromagnetic Heisenberg Hamiltonian (1.2), $v_s = \pi/2$ (see, e.g., Ref. !!!!), and hence $c = 1$.

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